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The mechanism of reactions of phosphorus-containing molecules with chloral: Density functional theory calculations

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Abstract

The most probable mechanisms of bimolecular interactions between a complex heterocyclic salicylic acid derivative, "phosphite," and chloral were for the first time studied by the density functional theory method. It was found theoretically that the reaction could develop in three different channels, (a) with six-membered heteroring opening and the formation of a seven-membered product and (b, c) as a Perkov-type reaction leading to (b) acyclic or (c) cyclic vinyl phosphates. The structures of the reagents, products, intermediates, and transition states were calculated with complete geometry optimization. All stationary points were identified by calculations of force constant matrices. For all transition states, intrinsic reaction coordinates were calculated. A comparison with the experimental data was performed. © 2008 Pleiades Publishing, Ltd.

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